ECE-656: Fall 2011

Lecture 41:

Transport in a Nutshell

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12/9/11

"the semiconductor equations"

Conservation Laws:

$$\nabla \bullet \vec{D} = \rho$$

$$\frac{\partial n}{\partial t} = -\nabla \bullet \left(\vec{J}_n / -q \right) + \left(G_n - R_n \right)$$

$$\frac{\partial p}{\partial t} = -\nabla \bullet \left(\vec{J}_p / \ q \right) + \left(G_p - R_p \right)$$

Constitutive Relations:

$$\vec{D} = \kappa \varepsilon_0 \vec{\mathcal{E}} = -\kappa \varepsilon_0 \vec{\nabla} V$$

$$\rho = q\left(p - n + N_D^+ - N_A^- \right)$$

$$\vec{J}_n = nq\mu_n \vec{\mathcal{E}} + qD_n \vec{\nabla} n$$

$$\vec{J}_p = pq\mu_p \vec{\mathcal{E}} - qD_p \vec{\nabla} p$$

$$R = f(n, p)$$

etc.

“the drift-diffusion equation”

$$\vec{J}_n = nq\mu_n \nabla F_n = nq\mu_n \vec{\mathcal{E}} + qD_n \vec{\nabla} n$$

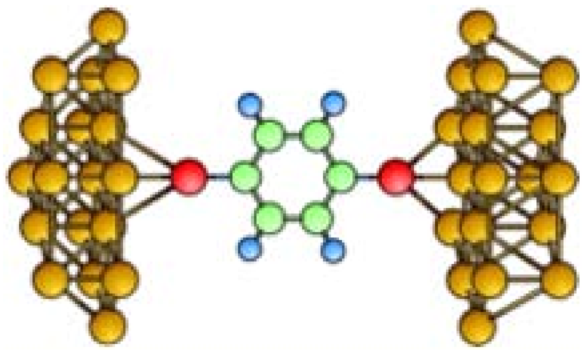
1) How is the DD equation derived?

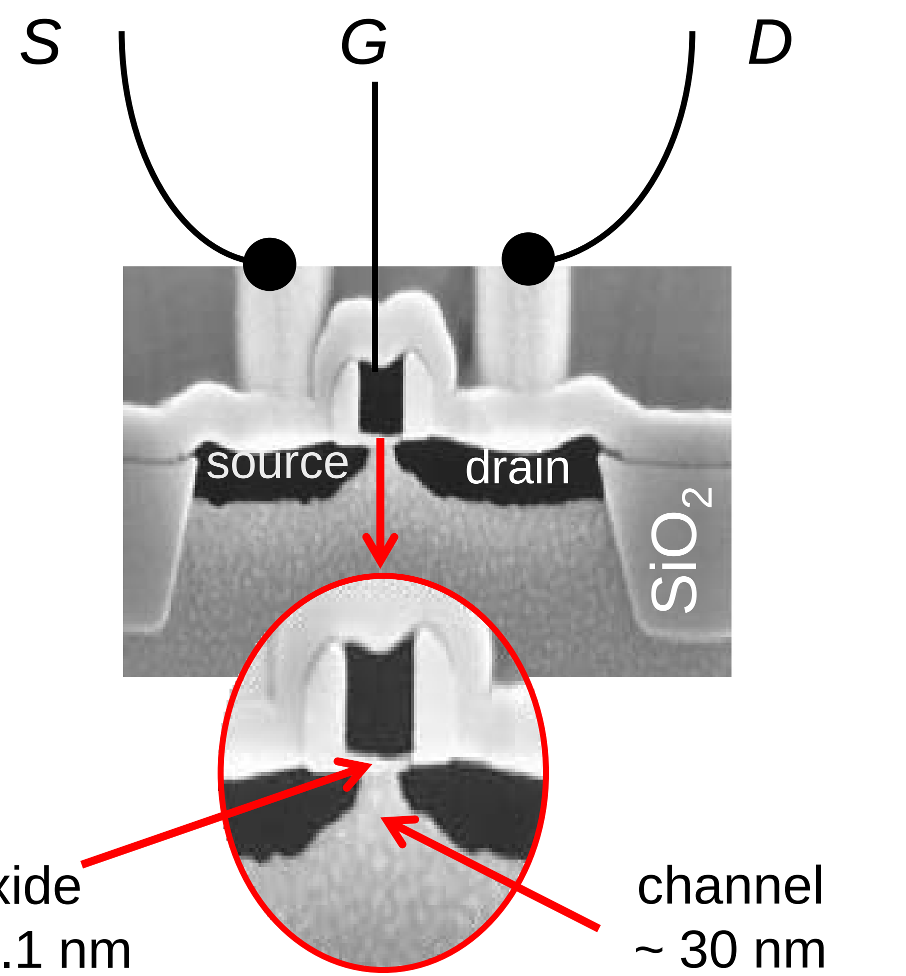
2) What determines the mobility and diffusion coefficient?

3) What physics does the DD miss?

4) How do we describe transport more rigorously?

bottom up approach





If we apply a bias between the two contacts, what current flows?

Landauer model

$$I = \frac{2q}{h} \int T(E) M(E) \left(f_1 - f_2 \right) dE$$

1) A difference in Femi functions cause current to flow

2) *M*(*E*) number of conducting channels at energy, *E*

3) *T*(*E*): transmission (0 < *T* < 1)

4) Important assumptions:

-contacts are “ideal” (absorbing, in equilibrium)
-inelastic scattering only in contacts

near-equilibrium conductance

$$I = \frac{2q}{h}\int T(E)M(E)\left(f_1 - f_2\right)dE$$

I > 0 when $V_2 > V_1$ because $f_1 > f_2$: $E_{F2} = E_{F1} - q\left(V_2 - V_1\right)$

When $(V_2 - V_1)$ is small, $f_1 \approx f_2 \approx f_0$ $\left(f_1 - f_2\right) \approx -\frac{\partial f_0}{\partial E}(qV)$

$$G = \frac{I}{V} = \frac{2q^2}{h}\int T(E)M(E)\left(-\frac{\partial f_0}{\partial E}\right)dE \qquad \frac{2q^2}{h} = \frac{1}{12.7\,k\Omega}$$

ballistic resistors (T = 1)

$$G = \frac{1}{R} = \frac{2q^2}{h}\int T(E)M(E)\left(-\frac{\partial f_0}{\partial E}\right)dE \qquad T = 1$$

For T_L = 0K or for strongly degenerate systems, $\left(-\partial f_0/\partial E\right) \approx \delta\left(E_F\right)$

$$G = \frac{2q^2}{h}M\left(E_F\right)$$

More generally:

$$G = \frac{2q^2}{h}\langle M\rangle \qquad \langle M\rangle \equiv \int M(E)\left(-\frac{\partial f_0}{\partial E}\right)dE$$

Density of states / Distribution of modes

Carrier densities are determined by the density of states.

Current flow is determined by the distribution of modes.

To determine $M(E)$:

1D: simply count the subbands

2D: $M(E)$ ~ width of the resistor, W

3D: $M(E)$ ~ cross-sectional area, A

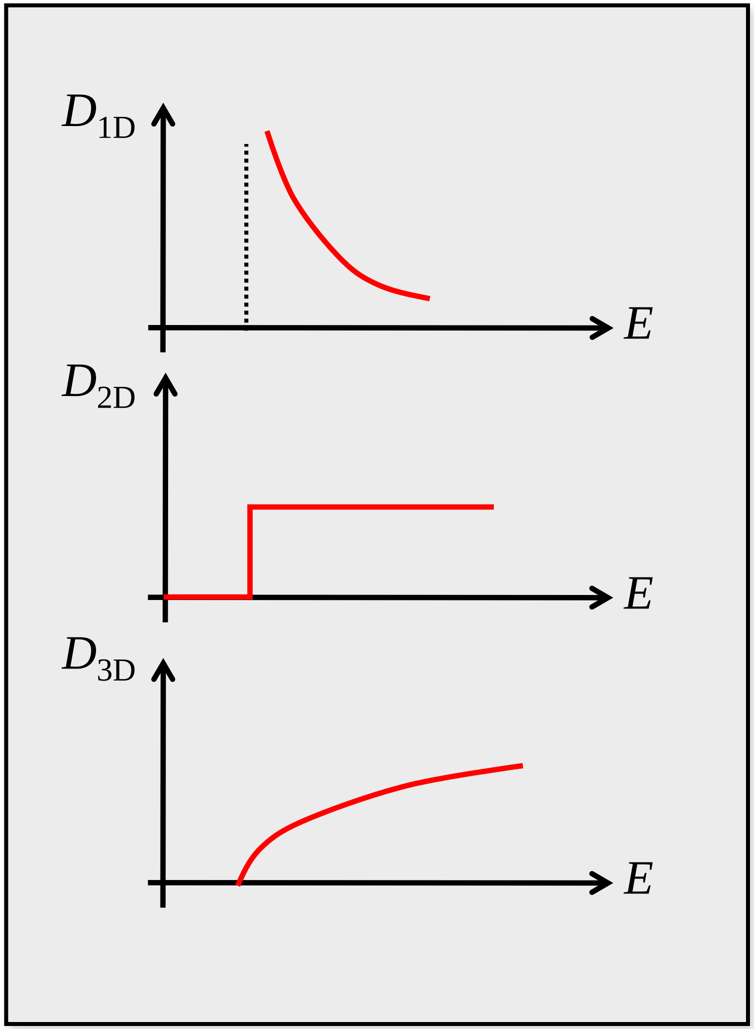
DOS depends on bandstructure and dimensionality

$$D_{1D}(E) = \frac{L}{\pi\hbar}\sqrt{\frac{2m^*}{(E-\varepsilon_1)}}\,\Theta(E-\varepsilon_1)$$

$$D_{2D}(E) = A\frac{m^*}{\pi\hbar^2}\Theta(E-\varepsilon_1)$$

$$D_{3D}(E) = \Omega\frac{m^*\sqrt{2m^*(E-E_C)}}{2\pi^2\hbar^3}$$

$$\left(E(k) = E_C + \hbar^2k^2/2m^*\right)$$



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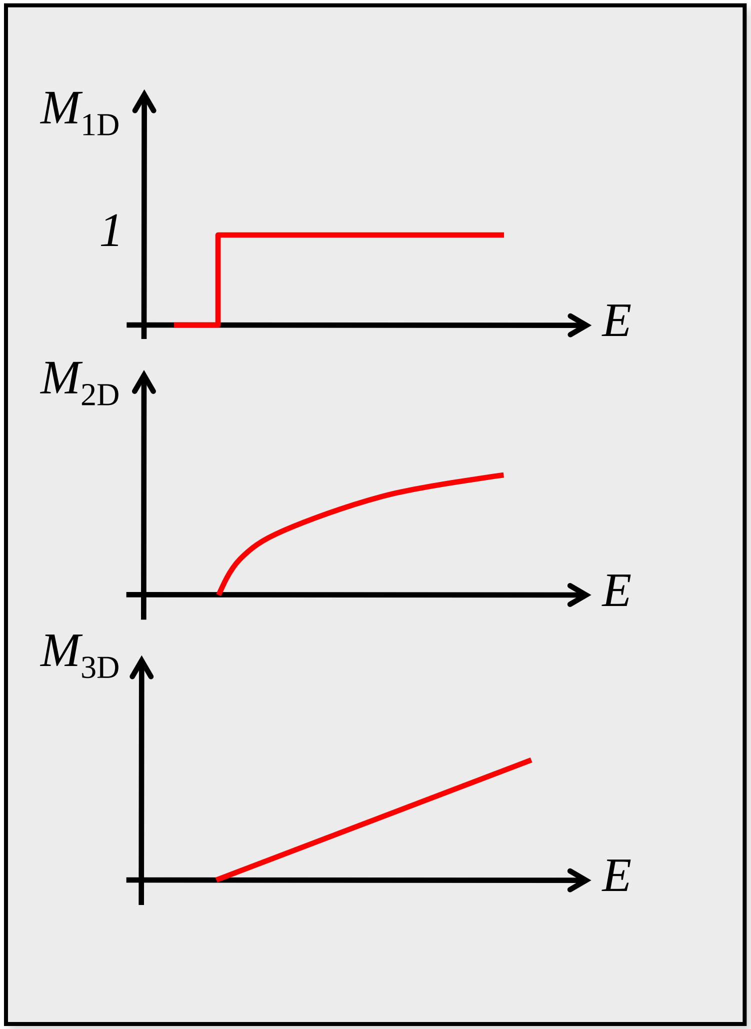
DOM depends on bandstructure and dimensionality

$$M_{1D}(E) = \Theta(E - \varepsilon_1)$$

$$M_{2D}(E) = W \frac{\sqrt{2m^*(E - \varepsilon_1)}}{\pi\hbar}$$

$$M_{3D}(E) = A \frac{m^*}{2\pi\hbar^2}(E - E_C)$$

$$\left(E(k) = E_C + \hbar^2 k^2 / 2m^*\right)$$



more generally

$$M(E) = \frac{h}{4}\left\langle \upsilon_x^+ \right\rangle D(E)$$

ballistic vs. diffusive

$$T(E) = \frac{\lambda(E)}{\lambda(E) + L}$$

λ is the "mean-free-path for backscattering"

$$G = \frac{2q^2}{h} T(E_F) M(E_F)$$

1) Ballistic : $\lambda >> L,\ T \approx 1$ $\qquad G = \frac{2q^2}{h} M(E_F)$

2) Diffusive : $\lambda << L,\ T << 1$ $\qquad G = \frac{2q^2}{h} M(E_F) \frac{\lambda(E_F)}{L}$

Explains why current ~ 1/*L* (1D), *W*/*L* (2D), and *A*/*L* (3D)

mobility and diffusion coefficient

$$G = \frac{2q^2}{h} \int T(E) M(E) \left(-\frac{\partial f_0}{\partial E} \right) dE \equiv nq\mu_n$$

For T = 0K:

$$\mu_n = \frac{q\tau(E_F)}{m^*}$$

For *non-degenerate conditions:*

$$\mu_n = \frac{D_n}{k_B T_L / q}$$

$$D_n = \frac{\upsilon_T \langle \lambda \rangle}{2} \qquad \upsilon_T = \sqrt{\frac{2 k_B T_L}{\pi m^*}}$$

Landauer and the DD equation

$$J_n = nq\mu_n \mathcal{E}_x + qD_n \frac{dn}{dx}$$

$$I_n = -\left\{ \frac{2q^2}{h} \int T(E) M(E) \left(-\frac{\partial f_0}{\partial E} \right) dE \right\} \Delta V$$

$$T(E) = \frac{\lambda(E)}{\lambda(E) + L} \approx \frac{\lambda(E)}{L}$$

$$J_n = \frac{I_n}{A}$$

$$\Delta F_n = -q\Delta V$$

$$J_n = \sigma_n \left. \frac{d(F_n/q)}{dx} \right|_{T_L} \qquad \sigma_n = \frac{2q^2}{h} \int \lambda(E) \frac{M(E)}{A} \left(-\frac{\partial f_0}{\partial E} \right) dE$$

driving forces for current flow

$$I = \frac{2q}{h} \int T(E) M(E) \left(f_1 - f_2 \right) dE$$

Anything that causes a difference in Fermi functions leads to current flow.

1) Differences in ***Fermi level*** (caused by differences in voltage)

2) Differences in ***temperature.***

For small difference (linear transport):

$$\left(f_1 - f_2 \right) \approx \left(-\frac{\partial f_0}{\partial E} \right) q \Delta V - \left(-\frac{\partial f_0}{\partial E} \right) \frac{\left(E - E_F \right)}{T_L} \Delta T_L$$

coupled current equations

$$I = G\Delta V + S_T \Delta T$$

$$I_Q = -T_L S_T \Delta V - K_0 \Delta T$$

$$\Delta V = RI - S\Delta T$$

$$I_Q = -\pi I - K_e \Delta T$$

$$G = \int G'(E)\,dE$$

$$G'(E) = \frac{2q^2}{h} T(E) M(E) \left(-\frac{\partial f_0}{\partial E} \right)$$

$$S_T = -\int \frac{(E - E_F)}{qT_L} G'(E)\,dE$$

$$K_0 = \int \frac{(E - E_F)^2}{q^2 T_L} G'(E)\,dE$$

$$S = \frac{S_T}{G}$$

$$K_e = K_0 - \pi S G$$

coupled current equations

$$J_x = \sigma \mathcal{E}_x - s_T \, dT_L / dx$$

$$J_x^q = T_L S_T \mathcal{E}_x - \kappa_0 \, dT_L / dx$$

$$\mathcal{E}_x = \rho J_x + S \frac{dT_L}{dx}$$

$$J_x^q = \pi J_x - \kappa_e \frac{dT_L}{dx}$$

(diffusive transport)

$$\sigma = \int \sigma'(E) dE$$

$$\sigma'(E) = \frac{2q^2}{h} \lambda(E) \frac{M(E)}{A} \left(-\frac{\partial f_0}{\partial E} \right)$$

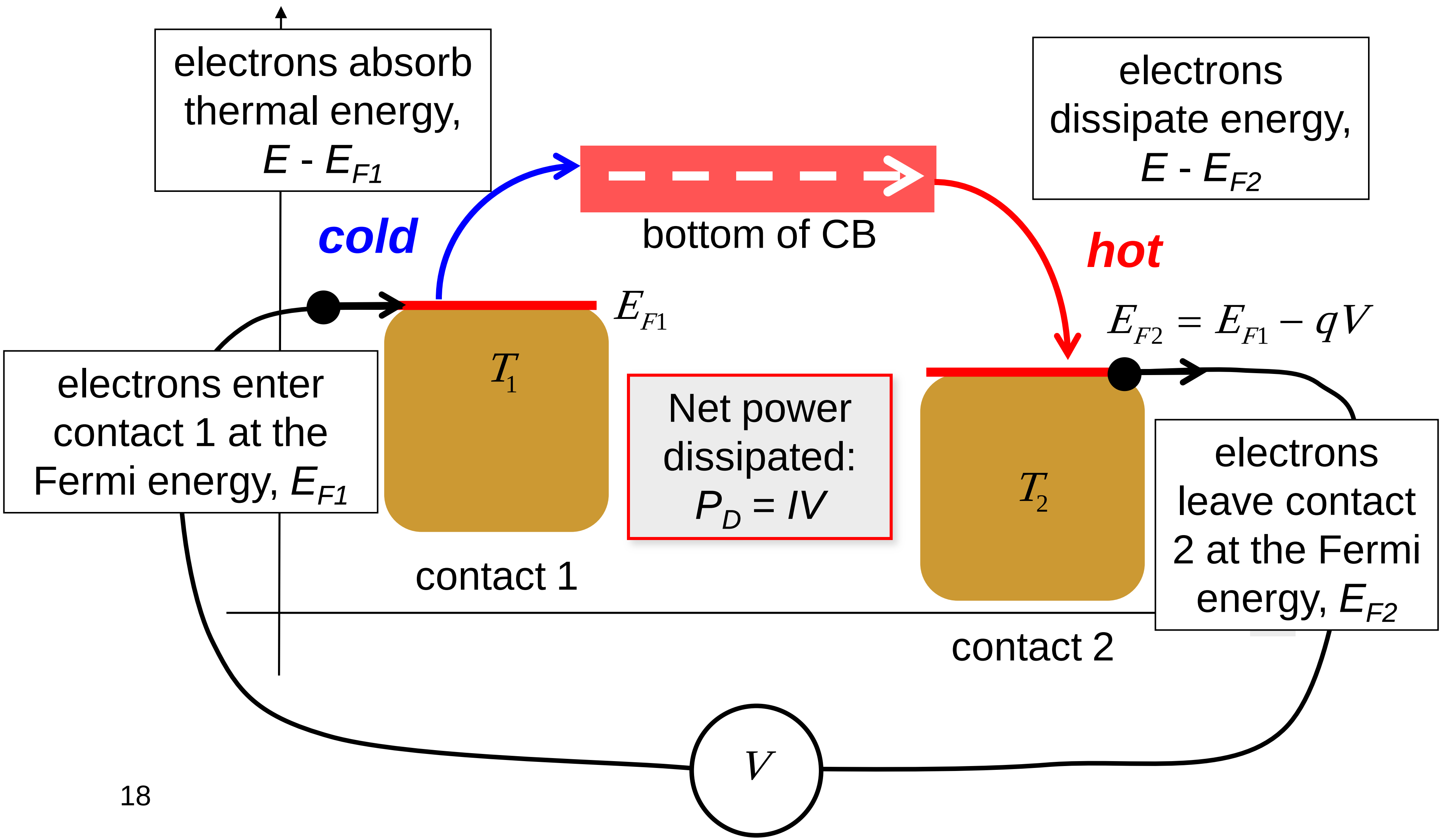
$$s_T = -\int \frac{(E - E_F)}{qT_L} \sigma'(E) dE$$

$$\kappa_0 = \int \frac{(E - E_F)^2}{q^2 T_L} \sigma'(E) dE$$

$$S = S_T / \sigma \qquad \pi = T_L S$$

$$\kappa_e = \kappa_0 - \pi S \sigma$$

physics of the Peltier effect



coupled current equations

$$\mathcal{E}_x = \rho J_x + S\frac{dT_L}{dx} \qquad J_x^q = \pi J_x - \kappa_e \frac{dT_L}{dx}$$

$$\sigma = \frac{2q^2}{h}\langle M\rangle\langle\langle\lambda\rangle\rangle$$

$$S = -\left(\frac{k_B}{q}\right)\left(\frac{E-E_F}{k_B T_L}\right)_{\text{ave}}$$

$$\pi = T_L S$$

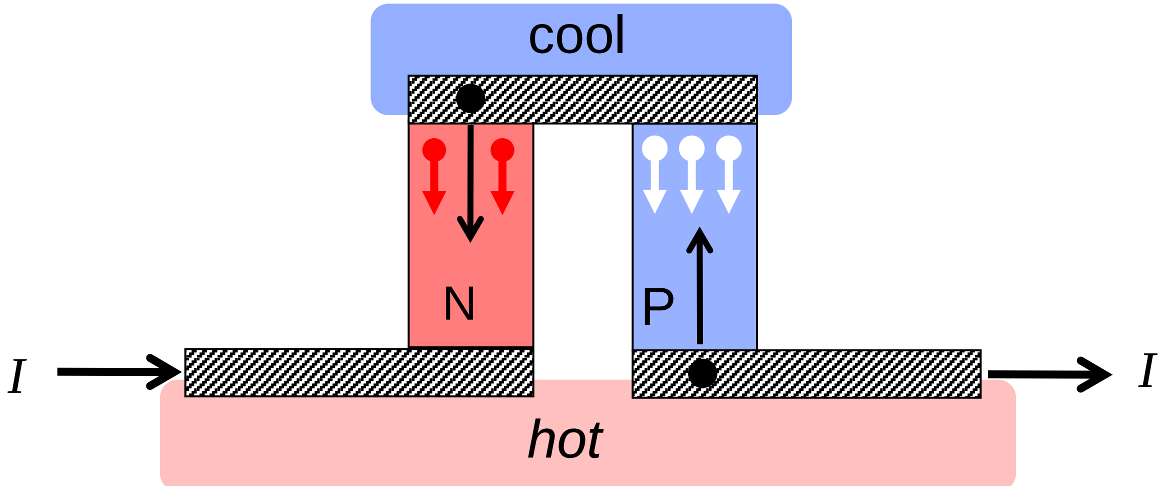
$$\kappa_n = \sigma_n T_L L$$

The Lorenz number depends on details of bandstructure, scattering, dimensionality, and degree of degeneracy, but for a constant mfp and parabolic energy bands:

$L \approx 2\left(\frac{k_B}{q}\right)^2$	$L \approx \frac{\pi^2}{3}\left(\frac{k_B}{q}\right)^2$
non-degenerate, 3D semiconductors	fully degenerate e.g. 3D metals

a “rule of thumb” not a “law of nature”

thermoelectric devices



$$ZT = \frac{S^2 \sigma \, T_L}{\kappa_e + \kappa_L}$$

$$|S| \downarrow \text{ as } E_F \uparrow$$

$$\sigma \uparrow \text{ as } E_F \uparrow$$

dimensionless figure of merit

the Boltzmann Transport Equation

1) near-equilibrium transport

2) hot-carrier transport in the bulk

3) non-local transport

The Boltzmann Transport Equation

semiclassical transport

$$\frac{d\left(\hbar\vec{k}\right)}{dt} = \vec{F}_e(\vec{r})$$

$$\vec{\upsilon}_g(t) = \frac{1}{\hbar}\nabla_k E\left[\vec{k}\left(t\right)\right]$$

$$\vec{r}\left(t\right) = \vec{r}\left(0\right) + \int_0^t \vec{\upsilon}_g(t')dt'$$

$$\frac{df}{dt} = \frac{\partial f}{\partial t} + \vec{\upsilon} \bullet \nabla_r f + \vec{F}_e \bullet \nabla_p f = \hat{C}f$$

$$\hat{C}f\left(\vec{r},\vec{p},t\right) = \sum_{p'} S\left(\vec{p}',\vec{p}\right) f\left(\vec{p}'\right)\left[1 - f\left(\vec{p}\right)\right]$$

$$-\sum_{p'} S\left(\vec{p},\vec{p}'\right) f\left(\vec{p}\right)\left[1 - f\left(\vec{p}'\right)\right]$$

solution to the BTE

$$\frac{\partial f}{\partial t} + \vec{\upsilon} \bullet \nabla_r f + \vec{F}_e \bullet \nabla_p f = \hat{C} f$$

1) Equilibrium: $\hat{C} f\left(\vec{r}, \vec{p}, t\right) = 0$

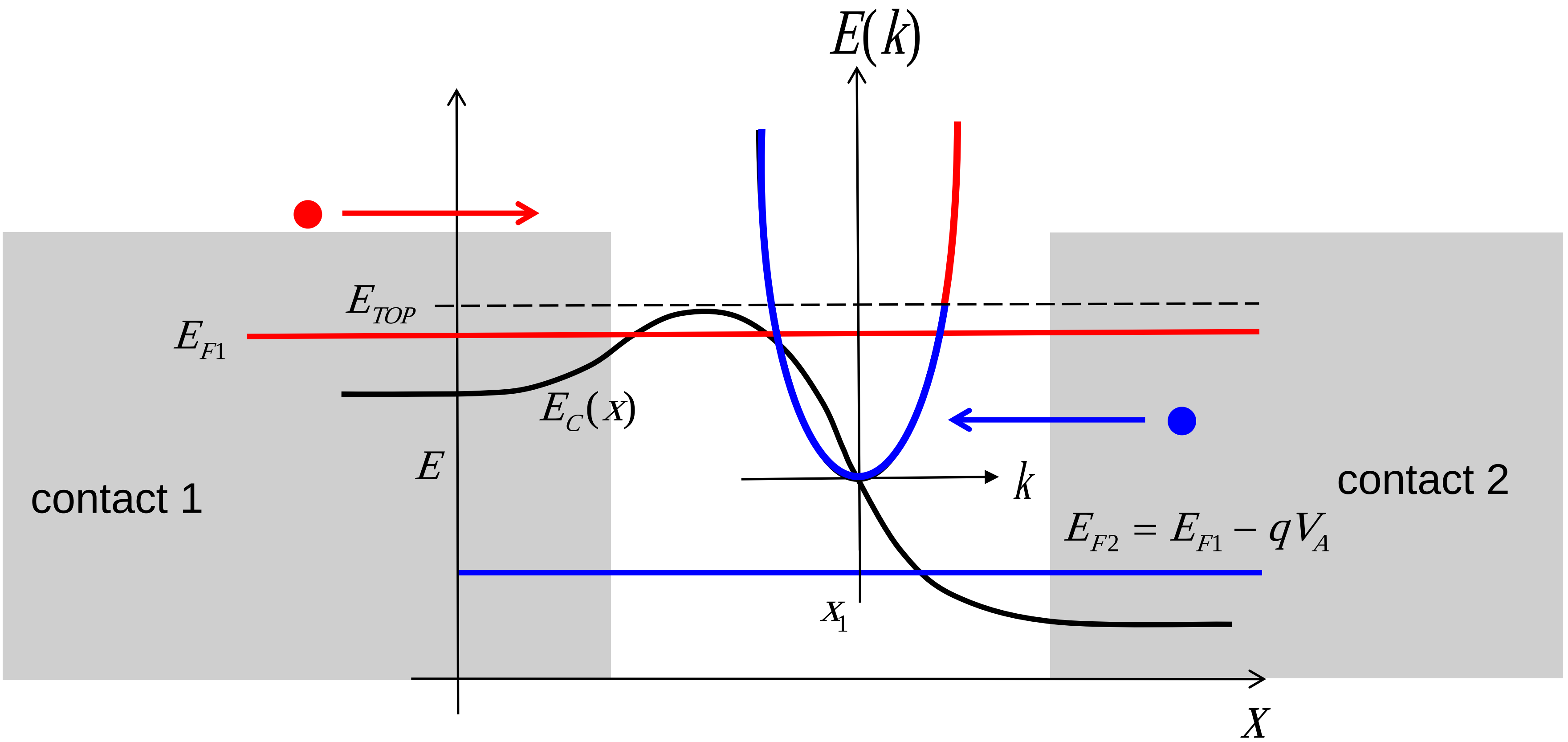
Fermi level and temperature are constant

2) Ballistic: $\hat{C} f\left(\vec{r}, \vec{p}, t\right) = 0$

Each state is populated according to an equilibrium Fermi function.

$$n(x) = \int D_1(x_1, E)\, f_0(E_{F1}) + D_2(x_1, E)\, f_0(E_{F2})\, dE$$

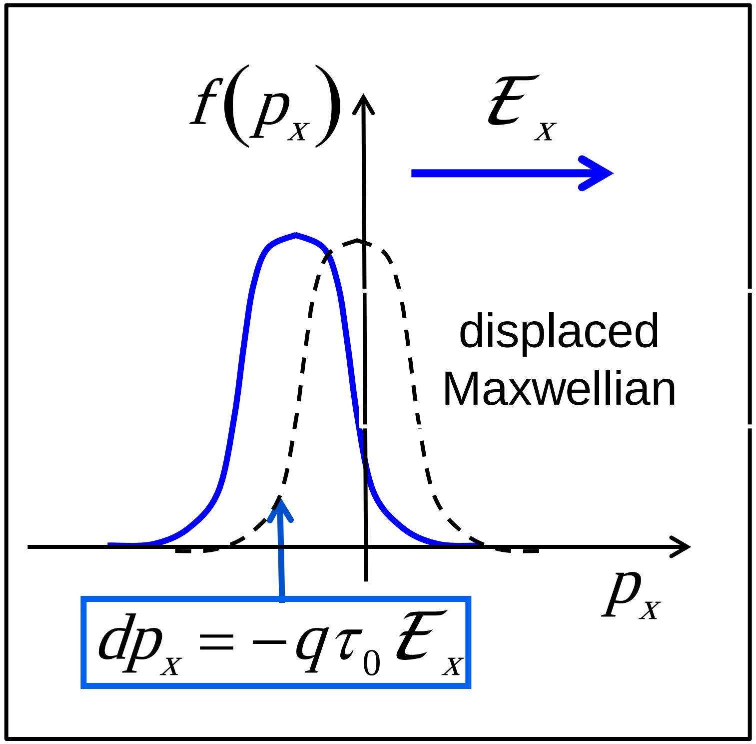
filling states in a ballistic device



relaxation time approximation

$$\frac{\partial f}{\partial t} + \vec{\upsilon} \bullet \nabla_r f + \vec{F}_e \bullet \nabla_p f = \hat{C} f = -\left(\frac{f(\vec{p}) - f_0(\vec{p})}{\tau_f} \right)$$

$$f(\vec{p}) = f_0(\vec{p}) + q \tau_f \mathcal{E}_x \frac{\partial f_0}{\partial p_x}$$ (no temperature or conc. gradients)



For diffusive, near-equilibrium transport, we get the same coupled current equations as from the Landauer approach.

BTE vs. Landauer

BTE:

-requires an $E(k)$ for the semi-classical treatment
-"hard" to apply boundary conditions
-works best in the diffusive regime
-B-fields readily incorporated
-anisotropic transport readily treated
-can be mathematically complex

Landauer:

-does not require an $E(k)$
-readily treats small devices with idealize boundary conditions
-works from the diffusive to ballistic regime
-physically transparent

B-fields

$$\frac{\partial f}{\partial t} + \vec{\upsilon} \bullet \nabla_r f + \vec{F}_e \bullet \nabla_p f = \hat{C} f = -\left(\frac{f(\vec{p}) - f_0(\vec{p})}{\tau_f} \right)$$

$$\vec{F}_e = -q\vec{\mathcal{E}} - q\vec{\upsilon} \times \vec{B}$$

$$J_i = \sigma_{ij}\left(\vec{B}\right)\mathcal{E}_j$$

$$\sigma_{ij}\left(\vec{B}\right) = \sigma_0 \begin{bmatrix} 1 & -\mu_H B_z \\ +\mu_H B_z & 1 \end{bmatrix} \quad \text{(2D)}$$

$$\vec{J} = \sigma_0 \vec{\mathcal{E}} - \sigma_0 \mu_H \vec{\mathcal{E}} \times \vec{B}$$

(Hall effect)

scattering

1) Landauer: $T(E)=\dfrac{\lambda(E)}{\lambda(E)+L}$

1) How is this equation derived?
2) How is mfp for backscattering related to the scattering time

$$\lambda(E)\propto \upsilon(E)\tau(E)$$

2) BTE: $\hat{C}f=\sum_{p'} S(\vec{p}',\vec{p})\,f(\vec{p}')\left[1-f(\vec{p})\right]-\sum_{p'} S(\vec{p},\vec{p}')\,f(\vec{p})\left[1-f(\vec{p}')\right]$

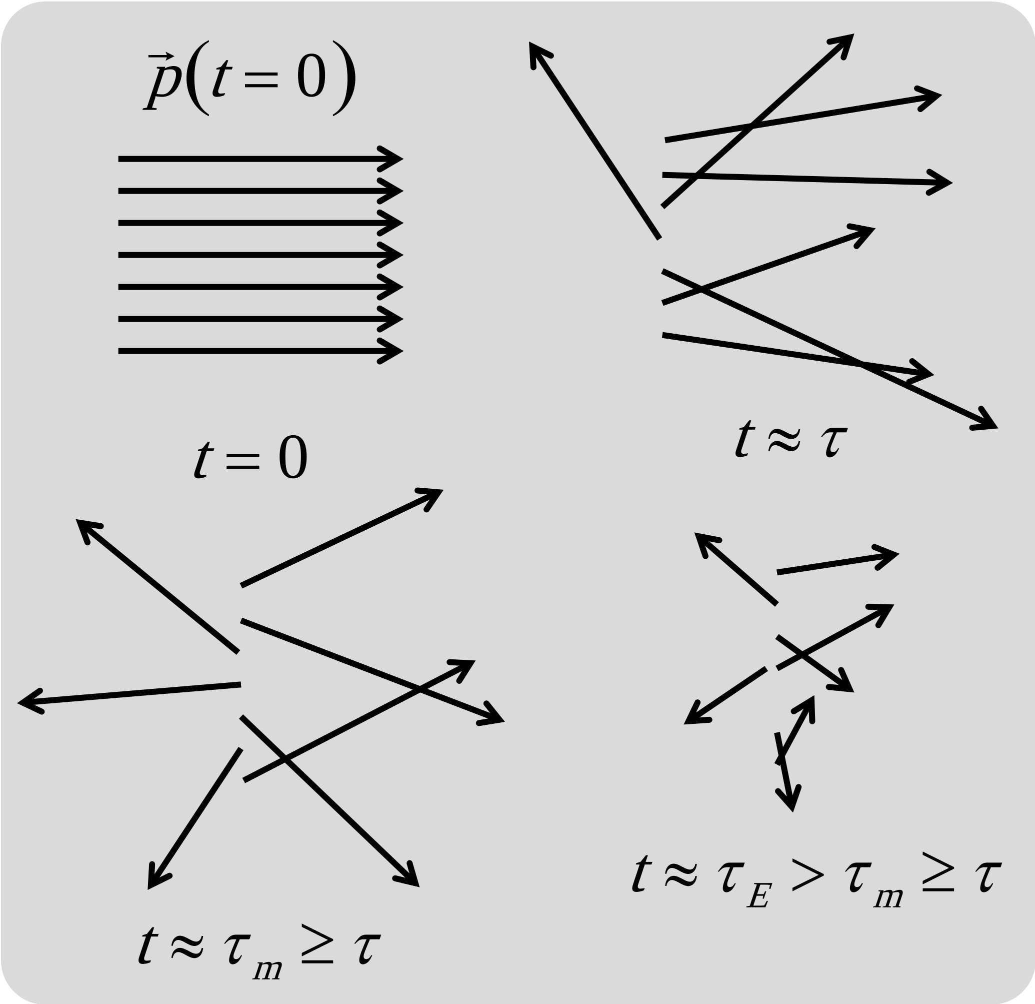
How is the transition rate, *S*(*p*,*p'*) computed?

characteristic times

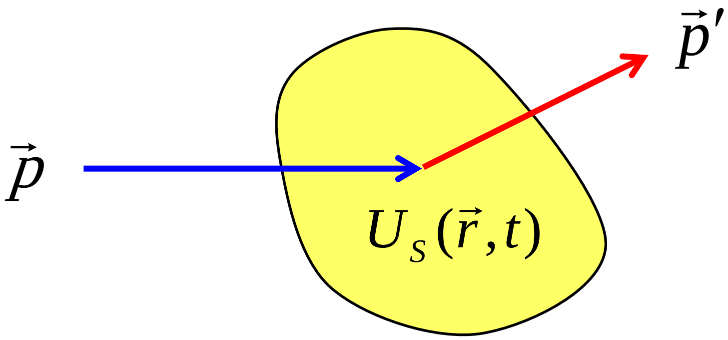
$$\frac{1}{\tau(\vec{p})} = \sum_{\vec{p}',\uparrow} S(\vec{p}, \vec{p}')$$

$$\frac{1}{\tau_m(\vec{p})} = \sum_{\vec{p}',\uparrow} S(\vec{p}, \vec{p}') \frac{\Delta p_z}{p_z}$$

$$\frac{1}{\tau_E(\vec{p})} = \sum_{\vec{p}',\uparrow} S(\vec{p}, \vec{p}') \frac{\Delta E}{E_0}$$



Fermi's Golden Rule



$$S(\vec{p},\vec{p}\,') = \frac{2\pi}{\hbar}\left|H_{p'p}\right|^2 \delta(E' - E - \Delta E)$$

$$H_{\vec{p}\,',\vec{p}} = \int_{-\infty}^{+\infty} \psi_f^* U_S(\vec{r})\psi_i d\vec{r}$$

$$E' = E_0 + \Delta E$$

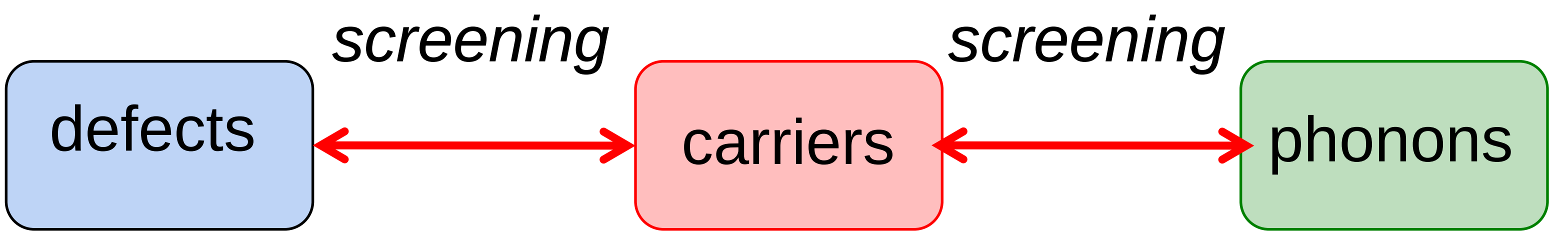
$\Delta E = 0$ for a static U_S

$\Delta E = \pm\hbar\omega$ for an oscillating U_S

$$\frac{1}{\tau(\vec{p})} = \sum_{\vec{p}\,'\uparrow} S(\vec{p},\vec{p}\,') \propto D_f(E)$$

For an electron with energy, *E*, its scattering rate is (often) proportional to the density of final states at energy, *E* (1D, 2D, 3D). Electrostatic interactions (II, POP), however, prefer small angle scattering.

scattering in semiconductors



- ionized impurities
- neutral impurities
- dislocations
- surface roughness
- alloy

- electron-electron
- electron-plasmon
- electron-hole

- intravalley
  - -ADP
  - -ODP
  - -POP
  - -PZ

- intervalley
  - -acoustic
  - -optical

near-equilibrium → far from equilibrium

The BTE also provides us with a way to treat transport under far from equilibrium conditions for which temporal and spatial transients may also occur.

moments of the BTE

The quantities of interest to device researchers are moments of the distribution function:

$$n_\phi\left(\vec{r},t\right)=\sum_{\vec{p}}\phi\left(\vec{p}\right)f\left(\vec{r},\vec{p},t\right)$$

These quantities satisfy a continuity equation:

$$\boxed{\frac{\partial n_\phi}{\partial t}=-\nabla\bullet\vec{F}_\phi+G_\phi-R_\phi}$$

A clear prescription for generating a continuity (or balance) equation exists, ***but*** simplifying the resulting equations for use in practice is an art.

example: the drift-diffusion equation again

$$\phi(\vec{p}) = (-q)\frac{p_i}{m^*} \qquad n_\phi(\vec{r},t) = J_{ni}(\vec{r},t)$$

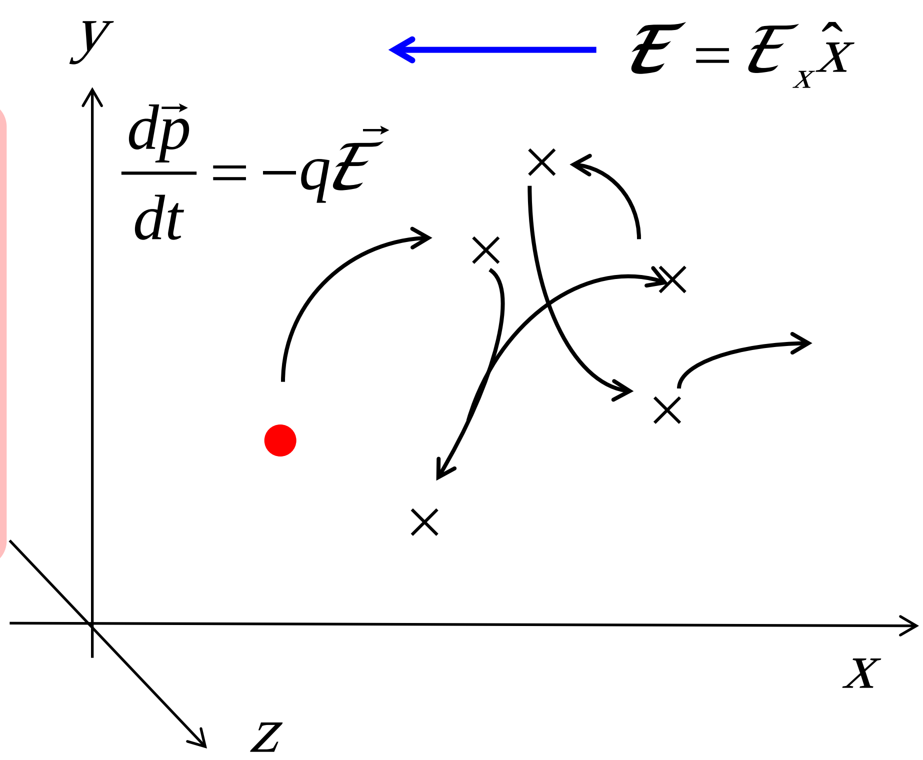
$$\vec{J}_n + \langle \tau_m \rangle \frac{\partial \vec{J}_n(\vec{r},t)}{\partial t} = nq\mu_n \vec{\mathcal{E}} + 2\mu_n \nabla \bullet \overleftrightarrow{W}$$

$$\mu_n = \frac{q\langle \tau_m \rangle}{m^*} \qquad W_{ij} = n\left\langle \frac{p_i \upsilon_j}{2} \right\rangle$$

$$J_{nx} = nq\mu_n \mathcal{E}_x + 2\mu_n \frac{d(nu_{xx})}{dx}$$

Monte Carlo simulation

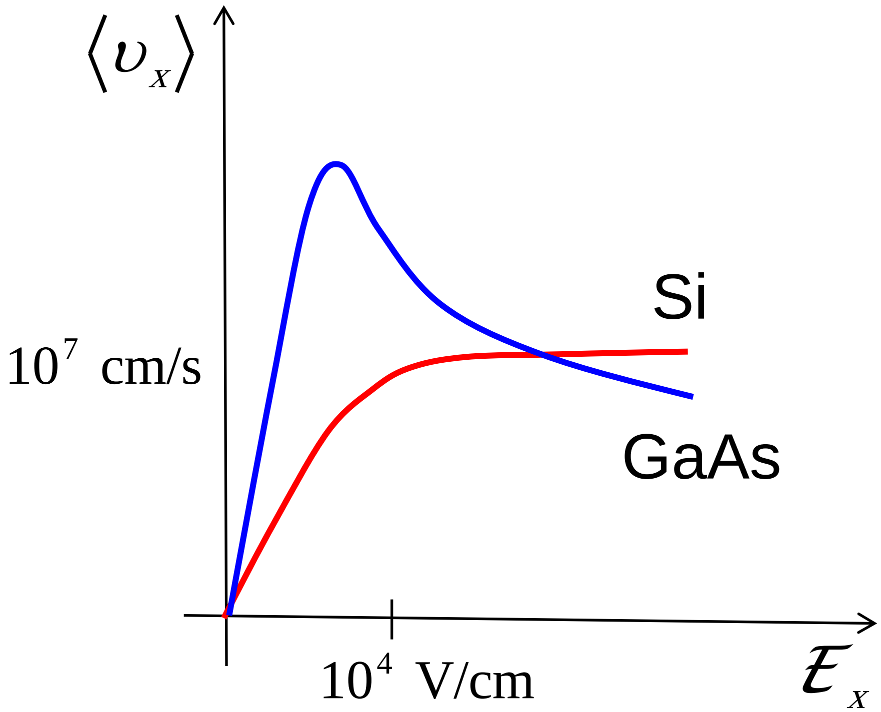
1) "free flight" for t_C seconds. r_1
2) update $E(t_C^-)$ and $r\ (t_C^-)$
3) identify collision r_2
4) update $E(t_C^+)$ and $p\ (t_C^+)$ r_3, r_4
5) Set t = 0 and repeat



1) free flights: semi-classical equations of motion

2) scattering: quantum mechanical transition rate $S(p,p')$

hot carrier transport

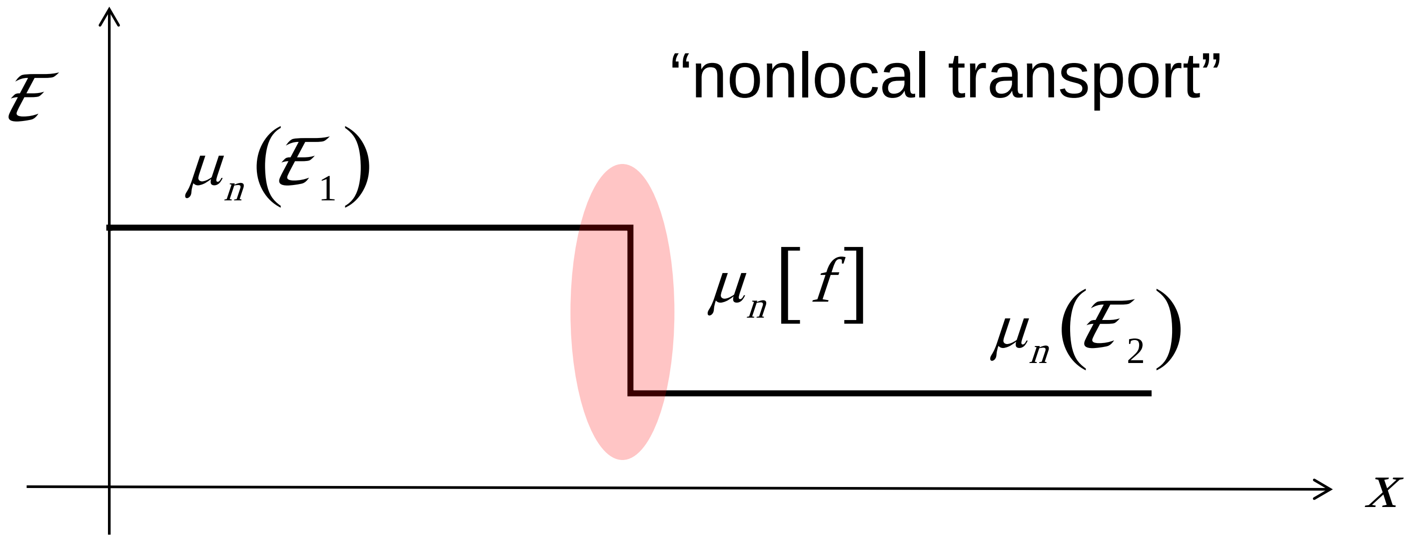


$$J_{nx}\mathcal{E}_x = \frac{n(u-u_0)}{\langle \tau_E \rangle}$$

$$\upsilon_{dx} = -\mu_n \mathcal{E}_x = -\frac{q\langle \tau_m \rangle}{m^*}\mathcal{E}_x$$

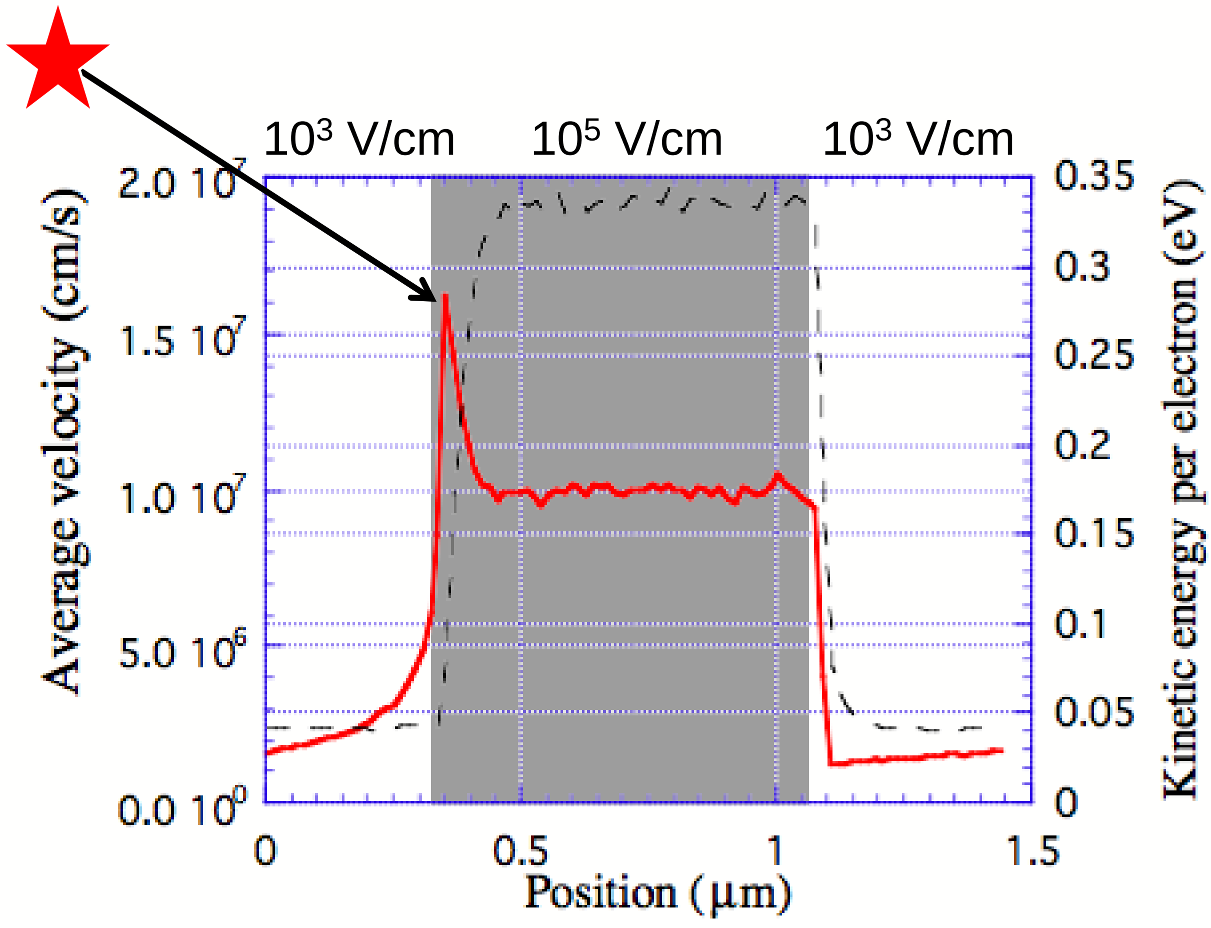
$\langle \tau_m \rangle \downarrow$ as $u \uparrow$

non-local transport



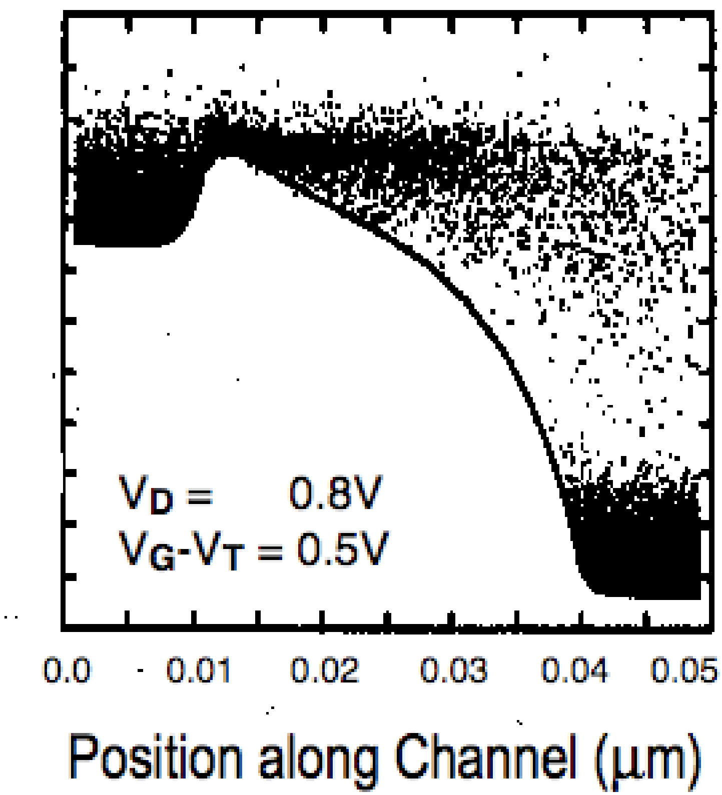
The concept of a field-dependent mobility applies <u>only</u> when the electric field changes slowly with position.

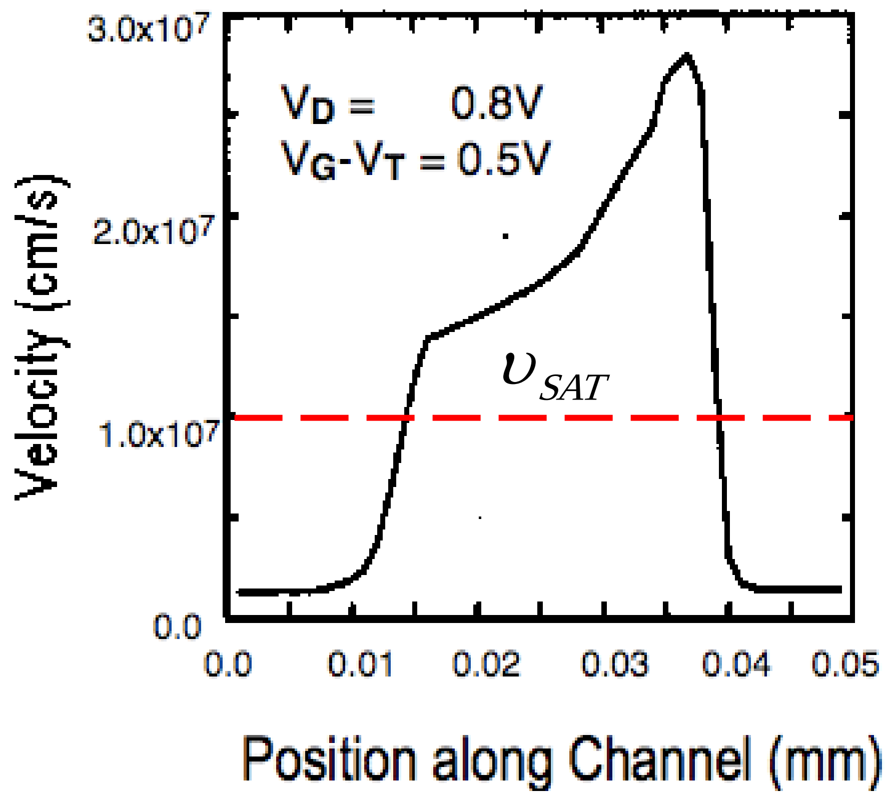
velocity overshoot



VO occurs in the presence of scattering when the energy relaxation time is longer than the momentum relaxation time.

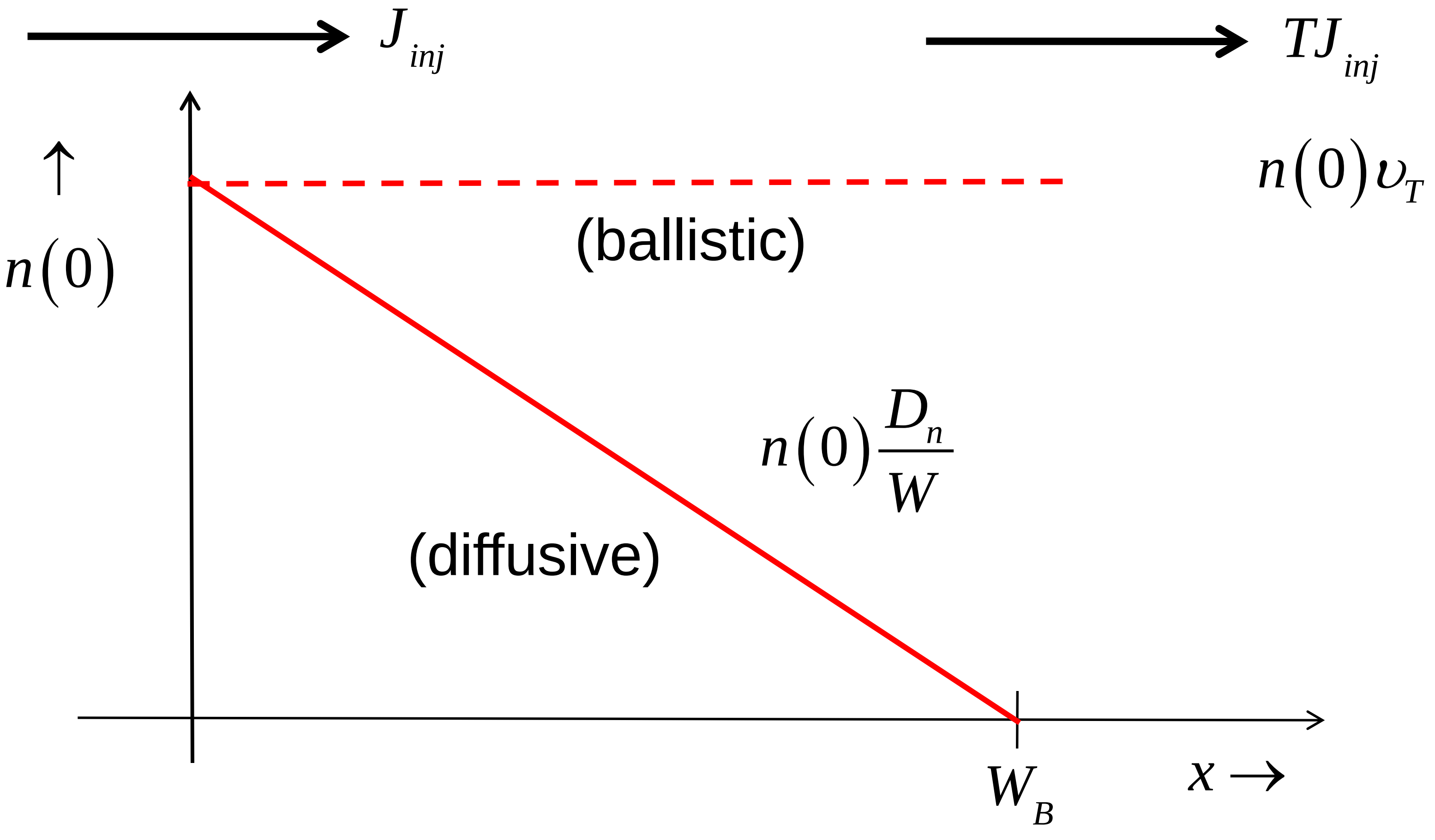
non-local transport in nanoscale MOSFETs





Frank, Laux, and Fischetti, IEDM Tech. Dig., p. 553, 1992

ballistic vs. diffusive transport



describing carrier transport

1) Landauer:

$$I = \frac{2q}{h} \int T(E) M(E) \left(f_1 - f_2 \right) dE$$

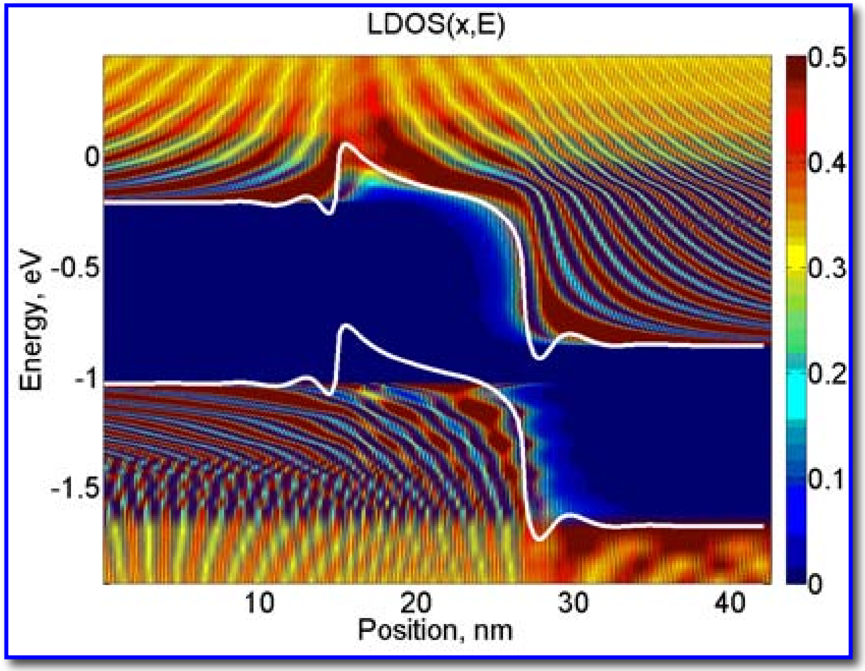
2) Boltzmann:

$$\frac{\partial f}{\partial t} + \vec{\upsilon} \bullet \nabla_r f + \vec{F}_e \bullet \nabla_p f = \hat{C} f$$

3) Quantum (NEGF):

$$[G(E)] = \left(E[I] - [H] - \left[\Sigma_{1,2} \right] - [\Sigma_S] \right)^{-1}$$

quantum transport



source + drain-injected LDOS in a carbon nanotube MOSFET

the drift-diffusion equation

$$J_n = nq\mu_n \mathcal{E}_x + qD_n \frac{dn}{dx}$$

1) Still describes transport in a very large number of cases

2) ECE-656 has taught you how to relate mobility and diffusion coefficient to material parameters and it suggests how we can engineer these parameters with strain and quantum confinement.

3) We have also learned about the assumptions underlying the DD equation – (e.g. slow variations in time and space).

4) We also learned that some problems cannot be treated by the DD equation – ballistic transport, non-local semiclassical transport, and quantum transport.

5) Finally, we learned some new techniques and how they related to the DD equations (Landauer approach, BTE, and an introduction to quantum transport.

wrap-up

With a good understanding of ECE-656, you should be prepared to solve any problem in transport that you encounter in your career.

(except percolation)